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Quantum mechanical ordering problem for observables which are linear in momentum

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Abstract. Starting with Segal's postulates for quantum mechanics, augmented by the postulate that the commutators of the free Hamiltonian with position observables are canonical, we prove that the quantum mechanical observable $Q(X)$, which corresponds to the function $C(X) \equiv X^i(q)p_i$ on phase space in classical mechanics, is equal to the anticommutator $\frac{1}{2}\{Q(X^i), Q(p_i)\}$. In coordinate free language, this means that $Q(\phi X) = \frac{1}{2}\{Q(\phi), Q(X)\}$ for any scalar field ϕ and any vector field X on the configuration space.

1. The algebra of quantum mechanical observables

Any classical dynamical system possesses a configuration space M. We suppose that M is a C^∞ manifold. The Hamiltonian $\frac{1}{2}g_{ij}(q)\dot{q}^i\dot{q}^j$ provides a metric g which makes M Riemannian. Denote by $T^{(s)}M$ the space of symmetric contravariant real C^∞ tensor fields S of valence $v(S) = s$ on M, $(s = 0, 1, 2 \ldots)$, and denote by $\mathscr{A}$ the direct sum

$$\mathscr{A} = \bigoplus_{s=0}^{\infty} T^{(s)}M.$$

To each $S \in T^{(s)}M$ corresponds the classical mechanical observable (CMO) or function on phase space, given in a local coordinate patch by

$$C(S) = S^{i_1 \ldots i_s}(q)p_{i_1}p_{i_2} \ldots p_{i_s}.$$

This function is homogeneous of degree s in momentum. The functions $C(S)$ form a Lie algebra under the Poisson bracket

$$\{C(S), C(T)\} = C([S, T]).$$

Here $[S, T]$ is a symmetric tensor field of valence $v(S)+v(T)-1$ called the Schouten concomitant of S and T, and the set $\mathscr{A}$ is a Lie algebra with the Schouten concomitant as Lie product. For further details see Sommers (1973) or Bloore (1975). We set up the quantization of this dynamical system as follows.

Following Segal (1960) we postulate that to each $S \in \mathscr{A}$ there is a quantum mechanical observable (QMO) $Q(S)$, and we consider the associative but not commutative algebra over $\mathbb{C}$ of polynomials in the symbols $Q(S)$, making the following identifications:

$$\text{P1} \qquad Q(cS) = cQ(S) \qquad c \in \mathbb{C}$$

$$\text{P2} \qquad Q(S+T) = Q(S)+Q(T)$$

$$\text{P3} \qquad Q(\phi\psi) = Q(\phi)Q(\psi) \qquad \phi, \psi \in T^{(0)}M$$

$$\text{P4} \qquad [Q(X), Q(\phi)] = -\mathrm{i}Q([X, \phi])$$

$$[Q(X), Q(Y)] = -\mathrm{i}Q([X, Y]) \qquad X, Y \in T^{(1)}M.$$

We also assume the map Q is faithful in the sense

$$\text{P0} \qquad Q(S) = 0 \Rightarrow S = 0.$$

As we shall see, these postulates do not prescribe uniquely $Q(\phi X)$ in terms of $Q(\phi)$ and $Q(X)$. To do this some extra condition is needed. We choose

$$\text{P5} \qquad [Q(g^{-1}), Q(\phi)] = -\mathrm{i}Q([g^{-1}, \phi]).$$

We denote by $\mathfrak{a}$ the resulting polynomial algebra of QMO. The purpose of this paper is to deduce from P0–P5 that

$$Q(\phi X) = \tfrac{1}{2}\{Q(\phi), Q(X)\}$$

where curly brackets round QMO denote the anticommutator. In a previous communication (Bloore and Underhill 1973) we gave a plausibility argument for this result. The rigorous proof is harder and more interesting than we expected so we think it is useful to publish it.

2. The function $F(\phi, X)$

We first observe that

$$Q(\phi X) = \tfrac{1}{2}\{Q(\phi), Q(X)\} + Q(F(\phi, X)) \tag{1}$$

where $F(\phi, X) \in T^{(0)}M$, since for any $\psi \in T^{(0)}M$, we have from postulates P2–P4

$$[Q(\psi), Q(\phi X) - \tfrac{1}{2}\{Q(\phi), Q(X)\}] = \mathrm{i}Q(\phi X\psi) - \tfrac{1}{2}\{Q(\phi), \mathrm{i}Q(X\psi)\} = 0.$$

Here we have used the notation $X\psi = [X, \psi] = X^i\partial\psi/\partial q^i$. It follows from P2 and P3 that $F(\phi, X)$ is linear in ϕ and X. In this section we prove F must satisfy the three conditions (3), (4) and (5). In the next section we deduce that $F = 0$.

It is evident from equation (1) that

$$F(1, X) = 0. \tag{2}$$

The requirement that $Q((\phi\psi)X) = Q(\phi(\psi X))$ implies that

$$F(\phi\psi, X) = \phi F(\psi, X) + F(\phi, \psi X). \tag{3}$$

If we take the commutator of equation (1) with $Q(Y)$ for an arbitrary vector field Y we obtain

$$YF(\phi, X) = F(Y\phi, X) + F(\phi, [Y, X]). \tag{4}$$

In obtaining equations (3) and (4) we have used the facts

$$\tfrac{1}{2}\{Q(\phi), \{Q(\psi), Q(X)\}\} = \{Q(\phi\psi), Q(X)\}$$
$$[Y, \phi X] = [Y, \phi]X + \phi[Y, X].$$

Postulate P3 gives

$$[Q(g^{-1}), Q(\phi\psi) - Q(\phi)Q(\psi)] = 0$$

which with P5 yields the condition

$$F(\phi, \operatorname{grad} \psi) + F(\psi, \operatorname{grad} \phi) = 0. \tag{5}$$

The postulates P0–P4 lead only to conditions (3) and (4). It may easily be checked that these conditions possess the solution

$$F(\phi, X) = \lambda X\phi \tag{6}$$

where λ is an arbitrary constant. We show in § 3 that this is the only possibility. Some extra postulate is thus needed to fix F, and we have taken P5. This leads to equation (5), which clearly requires $\lambda = 0$ if F is given by equation (6).

One can show that the vanishing of F is equivalent to an apparently stronger version of P5, namely

$$[Q(S), Q(\phi)] = -\mathrm{i}Q([S, \phi]) \qquad \forall S \in T^{(2)}M \tag{7}$$

but we reject making this our postulate because there seems less physical basis for equation (7), and also because P5 is strong enough.

3. Proof that F vanishes

We make the assumption that the value of the scalar field $F(\phi, X)$ at the point q of M depends only on the values and derivatives of ϕ and X at q: that is, we exclude non-local terms like

$$\int \mathrm{d}q' \int \mathrm{d}q'' f_{ij}(q, q', q'')\phi^{;i}(q')X^{j}(q'').$$

The most general form of F is then

$$F(\phi, X) = \sum_{l=1}^{L} \sum_{k=1}^{l} f_{a\, i_1 \ldots i_k\, i_{k+1} \ldots i_l} \phi^{;i_1 \ldots i_k} X^{a;i_{k+1} \ldots i_l} \tag{8}$$

where $L < \infty$ to ensure locality. The terms $k = 0$ in which ϕ is undifferentiated are excluded by equation (2). Repeated indices are summed from one up to the dimension n of the configuration space. The semicolon denotes covariant differentiation with respect to the Riemannian connection for the metric g. The coefficients f are the components of fixed tensor fields. Unsymmetrized combinations of covariant derivatives of order k of any tensor may be expressed in terms of its derivatives of order at most $k-2$ using the curvature tensor, so we define the coefficients f to be symmetric in $i_1 \ldots i_k$ and in $i_{k+1} \ldots i_l$ to avoid these ambiguities. These coefficients are then unique.

We substitute the form (8) into equation (3) and observe that the coefficients of the term

$$\phi^{;i_1 \ldots i_m} \psi^{;i_{m+1} \ldots i_k} X^{a;i_{k+1} \ldots i_l} \qquad 0 \leqslant m \leqslant k \leqslant l$$

are fully symmetric in $i_1 \ldots i_m$, in $i_{m+1} \ldots i_k$ and in $i_{k+1} \ldots i_l$. They may therefore be equated. (This is *not* the case for equation (4); there the indices have to be symmetrized by us.) Doing this yields the equation

$$\delta_{m0} f_{a\, i_1 \ldots i_k i_{k+1} \ldots i_l} + \binom{l-m}{k-m} f_{a\, i_1 \ldots i_m i_{m+1} \ldots i_l} = \binom{k}{m} f_{a\, i_1 \ldots i_k i_{k+1} \ldots i_l}.$$

In the cases $m = 0$ and $m = k$ this equation is an identity. For $0 < m < k \leqslant l$ it gives

$$\binom{l}{m}^{-1} f_{a.i_1 \ldots i_m i_{m+1} \ldots i_l} = \binom{l}{k}^{-1} f_{a\, i_1 \ldots i_k i_{k+1} \ldots i_l}$$

which implies that

$$f_{a.i_1 \ldots i_k i_{k+1} \ldots i_l} = \binom{l}{k} h_{a.i_1 \ldots i_l}$$

where h is fully symmetric in $i_1 \ldots i_l$. Thus the general solution of equation (3) is

$$\begin{aligned} F(\phi, X) &= \sum_{l=1}^{L} h_{a\, i_1 \ldots i_l} \sum_{k=1}^{l} \binom{l}{k} \phi^{;i_1 \ldots i_k} X^{a;i_{k+1} \ldots i_l} \\ &= \sum_{l=1}^{L} h_{a.i_1 \ldots i_l}[(\phi X^a)^{;i_1 \ldots i_l} - \phi X^{a;i_1 \ldots i_l}] \end{aligned} \qquad (9)$$

where the h are arbitrary tensors symmetric in $i_1 \ldots i_l$.

We now show that the form (9) satisfies equation (4) only if $L = 1$ and

$$h_{a\, i_1} = \lambda g_{ai_1} \qquad (10)$$

so that F is given by equation (6). If we substitute equation (9) into equation (4) and collect together the terms which involve the highest ($=L$th) derivatives of the components of Y we obtain

$$Y^{\alpha;i_1 \ldots i_L} X^a \phi^{;\beta}[-g_{\alpha\beta} h_{a.i_1 \ldots i_L} + L g_{ai_1} h_{\alpha.\beta i_2 \ldots i_L}].$$

The symmetrized part cannot be cancelled by lower order terms, so we may deduce that

$$g_{\alpha\beta} h_{a.i_1 \ldots i_L} = L h_{\alpha\, \beta(i_2 \ldots i_L} g_{i_1)a}$$

where bracketed indices are symmetrized. The $\alpha\beta$ trace of this equation is

$$n h_{a\, i_1 \ldots i_L} = L h^{\alpha}{}_{\alpha(i_2 \ldots i_L} g_{i_1)a} \qquad (11)$$

where $n = \dim M$. The ai_1 trace of *this* equation is

$$(L-1) h^{\alpha}{}_{\alpha i_2 \ldots i_L} = 0.$$

Hence for $L > 1$, by equation (11),

$$h_{a\, i_1 \ldots i_L} = 0.$$

Thus equation (9) reduces to at most

$$F(\phi, X) = h_{a.i_1} \phi^{;i_1} X^a.$$

Substituting this into equation (4) gives, for all ϕ, X, Y

$$\phi^{;i_1}\{X^a Y^b h_{a.i_1;b} + X^a Y^{b;c}(h_{b\, i_1} g_{ac} - h_{a\, c} g_{bi_1})\} = 0$$

which holds if and only if $h_{a i_1}$ is given by equation (10). Hence equation (6) is the only possibility for F, in which case equation (5) specifies that $F = 0$.

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